

Crystal Chemistry of Trace Metals in Cementitious Hydraulic Binders	X23A2
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I. Moulin, J. Rose, A. Masion, E. Doelsch, J-Y. Bottero (CEREGE) and P.M. Bertsch (AACES-SREL)

The assessment of environmental risks linked to the use of cement materials containing trace metals (Pb, Zn, Cr, Cu) and the prediction of the long term behavior require the knowledge of their physico-chemical stability, i.e. their local scale environment (speciation) in the three cement phases $3\text{CaO}.\text{SiO}_2$ (C3S), $4\text{CaO}.\text{Al}_2\text{O}_3.\text{Fe}_2\text{O}_3$ (C4AF) and $3\text{CaO}.\text{Al}_2\text{O}_3$ (C3A). This investigation was conducted using the X23A2 beamline of the NSLS.

Preliminary sorption experiments showed that the C3S and C4AF cement phases have a high- whereas the C3A phase showed a lower affinity for Zn. In all 3 phases Zn has a four-fold coordination. Modeling of the second atomic shell around Zn allowed to give some explanation for the differential Zn affinity of the cement phases. For both C3S and C4AF phases, Zn is incorporated into the hydrated cement phase matrix and consequently less subjected to leaching. Zn is surrounded by 0.7 Si at 3.07 Å and 0.4 Ca at 3.00 Å in the C3S phase and by 2.4 Zn at 3.40 Å and 2.7 Fe at 3.5 Å in the C4AF phase. In the "low affinity" C3A phase, the Zn coordination is identical to the hydroxyzincate standard (2 Zn at 3.44 Å; 2 Ca at 3.78 Å), showing that precipitation of hydroxyzincate particles occurred during the hydration of Zn-C3A.

In the case of lead and C3S phase, only Pb-O distances were detected suggesting that lead prevents the hydration of the C3S by adsorption onto the surface. In the hydrated phase, Pb binds to Si, which correlates well with Si NMR data. In the C4AF phase, Pb-Fe contribution were detected. This was expected from the higher affinity of Pb compared to the other cement phase pointed out by sorption experiments.